Theoretical Method for the Study of Plasmon Generation in Hybrid Multilayer-Optical Fiber Structures

Óscar Esteban, María-Cruz Navarrete, and Agustín González-Cano

***Abstract*—A theoretical method is presented for the determination of the behavior of devices based on the deposition of multilayer structures on polished optical fibers. Plasmon generation in metallic layers is modeled. The method is based on the Rayleigh expansion of the electric fields and permits us to determine their distribution over the whole structure by an application of boundary conditions. Once the distribution is known, the power transmitted by the fiber can be computed as a function of the geometrical and refractive parameters of the device. The method is versatile and can be used as a theoretical tool for the design of devices of that type used for many different purposes. We present real experimental results obtained with an operative sensor that agree with the theoretical predictions of our technique and prove its suitability.**

***Index Terms*—42.81 (optical fibers), 42.81.P (fiber-optic sensors), PACS numbers: 73.20.M (surface plasmons).**

I. Introduction

THE PROBLEM of the theoretical modeling of complex light-guiding structures is a complicated one, since no analytical solution can be obtained when the usual symmetry conditions are not fulfilled and the most common approaches, such as modal decomposition in substructures, are not suitable in many cases. One example of these complex structures may be the devices based on D-fibers (optical fibers with the cladding polished up to a few microns to permit interaction with the evanescent field of the guided modes of the fiber). This kind of fiber has been used in many devices, such as couplers, polarizers, sensors, etc. In many cases, one or more layers of different materials are deposited on the polished fibers, thus forming what we can call a *hybrid* structure in which we have, at least, two different guiding structures (namely, the optical fiber and the plane layers) which should not be treated separately [1]–[6].

For those hybrid structures, we cannot assume any simple symmetry, in principle, and a modal decomposition in the different substructures (the multilayer and the fiber) and the subsequent study of the behavior of the system in terms of mode coupling [7], [8] do not always provide good results and the agreement with experimental measures is usually poor. Modal decomposition, in fact, requires the separability of the two structures to be of real profit, because only in that case can we work with the usual theoretical expressions for the modes of cylindrical or plane waveguides. Once the different sets of modes are calculated, we can consider the problem of the energy transfer between substructures as one of coupling. In any case, we do not really have a global depiction of the structure, and we rely in "canonical" solutions, as the modes are, to solve a problem which can be considerably more complex. The result is, as we have said before, disagreement between theory and experiment.

One common option to overcome the problem of the lack of symmetry is to substitute the cylindrical optical fiber for the equivalent plane guide [9]. A number of techniques has been proposed based on that approach, some of them using geometrical approximations [5], [10]. It remains, however, a problem that the depiction is still made in terms of modes and that we must first assume an approximation which cannot be too adequate.

The presence of metallic layers and the possible excitation of surface plasmons on them adds a new, different complication. Although we can treat plasmons as guided modes, the search of the propagation constants associated to them is not easy, since we must work in the complex plane. However, it is quite common to use surface-plasmon resonance as a basis for many devices, especially sensors [3], [4], [11]–[13]. These sensors are used for different types of measurements. The most common ones are based directly or indirectly on the dependence of the response of the devices to changes of the refractive index of the surrounding medium. The authors have used D-fibers with a double layer (metal-dielectric) to measure salinity in sea water [4]. In that case, the presence of a double layer was necessary to tune the response of the sensor to the required refractive index. In this way, operative sensors based on surface plasmon resonance are not always constituted by a single metallic layer deposited on a fiber. The theoretical study of these devices, which are hybrid waveguide structures and also incorporates metallic layers is the most difficult one, and the modal-decomposition-based methods are not well suited for this study.

However, it is precisely for that kind of structure that one needs good theoretical knowledge, not only because the study

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of the field propagation in the devices is interesting by itself, but also because it is very important to have a method for predicting the behavior of the devices as a tool for their design, since we are always obliged to select the parameters of the structure in such a way that the response of the sensor is the best one for the measures that we desire.

If we use modal decomposition to model the structures, we can, at best, obtain a rough estimation of the coupling point for the substructures, but not a complete account of the response of the system on the whole operation range. We could consider exact methods in which the propagation equations for the electromagnetic field are solved, but this is really difficult for the kind of structures in which we are interested. In this way, the ideal method could be one which is not based on modal decomposition, but is still simple enough so that it can be used in the design stage of the device, when the constructive parameters of the sensor are to be defined.

In a recent work [14], the authors have presented a method which can fulfill these requirements of accuracy and simplicity. It is, in fact, a novel approach for the theoretical modeling of hybrid guiding structures, and has been successfully applied to quite simple structures (a D-fiber plus a single metallic layer). The method is not based on any modal decomposition or mode-coupling calculations. It is based on the Rayleigh expansion of the electric field [15] and allows us to calculate the field distribution in the different regions of the complete structure and to determine the power transmitted by the fiber once the interaction with the deposited layers has taken place, thus modeling the response of the sensors which are based in this kind of hybrid guides.

In [14], the method is presented and applied to a simple case. In this paper, we generalize the method, depicting it in a more rigorous way, and, more importantly, we show its suitability for the theoretical study of more complex structures, namely, D-fibers with double layers (metallic plus dielectric). Passing from only one metallic layer to a double layer with two materials of different behavior is not a trivial step. It is in this kind of complex structures where our method proves its interest, and, as it can be seen in the following paragraphs, we have obtained a good agreement between the theoretical predictions and the experimental results obtained with a real, operative sensor. In this way, the method can be, in principle, applied to any hybrid guiding structure, providing a complete depiction of the behavior of the system, for any choice of the constructive parameters of the structure, including the prediction of plasmon generation in the metallic layers. The simplicity and versatility of the method make it also applicable to many other different situations in which a calculation of the distribution of the electromagnetic field is required.

II. Depiction of the Method

The basic features and assumptions of the method are depicted in [14]. We summarize here the most important points, because, as we said before, the application of the technique to a complex structure is not a trivial task, and some considerations must be taken into account.

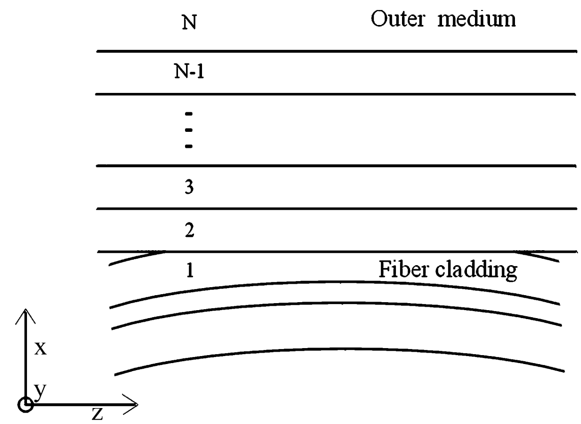

Fig. 1. Scheme of the studied structure. A series of planar layers of different dielectric or metallic layers are deposited on a D-fiber, with a polished cladding. The notation used in this paper is shown; the last medium is what we consider "outer medium" and is taken as semi-infinite and labeled with the N subscript.

A. Outline

The structures that we study can be represented by the scheme of Fig. 1. A plane multilayer with both dielectric and metallic materials is deposed on a D-fiber. The method can be used for any number of layers and we give a general depiction for a system with N different layers that we will design by a subscript $m = 1, 2, \ldots, N$, where 1 denotes the cladding of the fiber, taken as the first layer, and N is the medium that surrounds the structure. For each region of the structure, we will take, as defining parameters, its thickness d_m and its refractive index n_m.

We have schematized the method in Fig. 2. Our goal is not only to predict the appearance of surface plasmons, but also to calculate the distribution of the field in any region of the hybrid structure. Each of these regions (layers and fiber) will have a Rayleigh expansion of the field, and we will apply the boundary conditions to relate the distributions. Once we have determined these distributions, we will be able to estimate the losses in the power transmitted by the fiber due to the transfer of energy from the fiber to the multilayer. We can perform these calculations for any choice of the parameters of the structure (thickness and refractive index). In the specific case of a refractive-index sensor, we can, for instance, consider how the variation of the refractive index of the surrounding medium can affect to the response of the sensor by iterating the calculation for a desired number of different values of that refractive index.

B. Calculation of Initial Field Distribution

To proceed with the method, we need to first define the initial field distribution. We take it as the evanescent field which would correspond to a cylindrical single-mode optical fiber with known geometrical and refractive characteristics. The polishing of the cladding permits this evanescent field to interact with the deposited structure. The perturbation introduced by the polishing in the form of the "canonical" evanescent field is not taken into account, since, as we have proved in our previous work and confirm in this, the results obtained are good enough within this approximation. It is taken into account, however, the

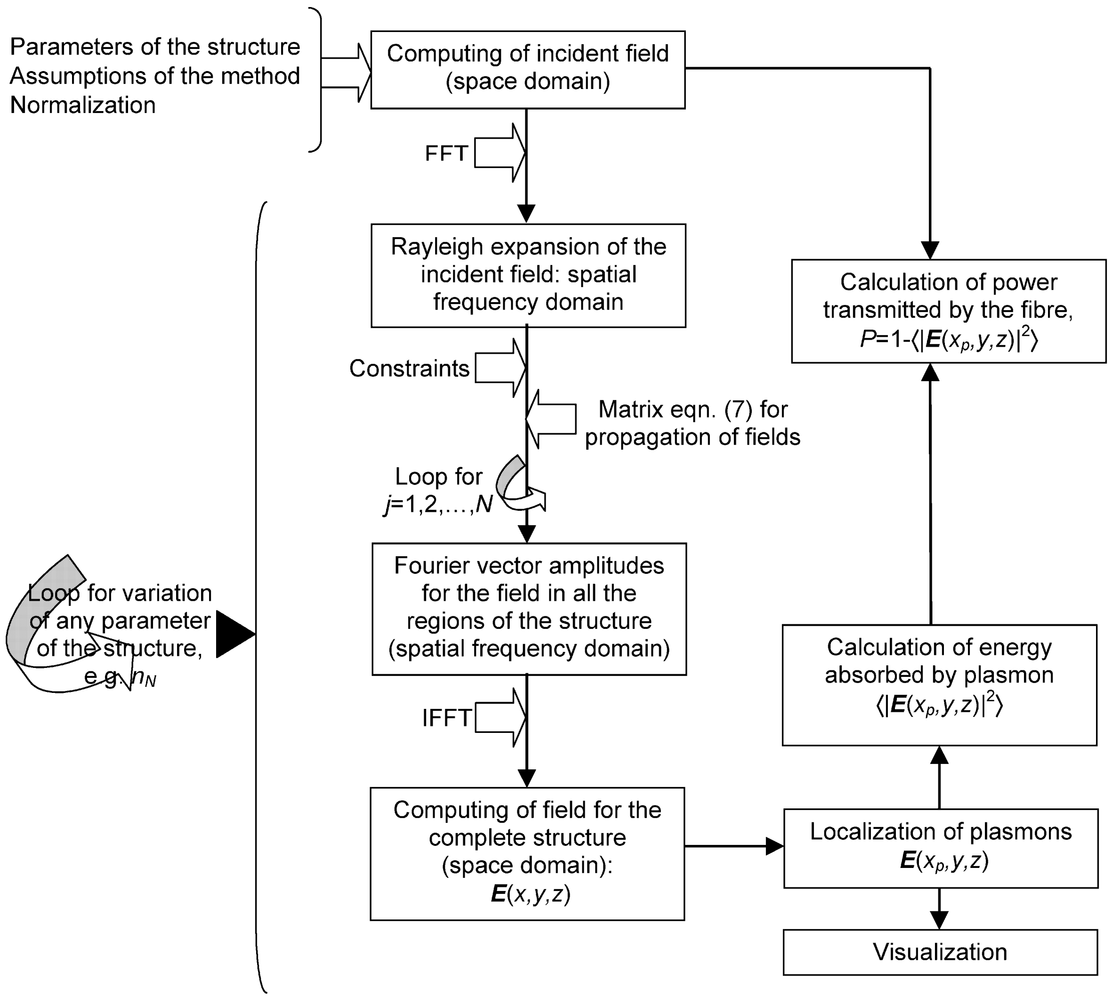

Fig. 2. Block diagram of the theoretical method.

fact that the remaining thickness of the cladding is not a constant one, because of the cylindrical form of the fiber. We must use this thickness as an initial parameter and it must be estimated from the geometrical characteristics of the polished area and the values of the attenuation [16]. These parameters, which can be experimentally determined, give us a value for the curvature radius of the fiber in the region of the deposition. We must remember that, as it is illustrated in Fig. 1, the fiber is curved to be polished: it is this curvature that we must consider. Assuming this curvature, we can calculate the separation from the core to the first plane layer $m = 2$ (i.e., the thickness of the "layer 1," corresponding to the remaining cladding) by simple geometrical calculations as a function of the distance of propagation z. The thickness is given by

$$D(z) = d + R_1 - \sqrt{R_1^2 - z^2} \tag{1}$$

with d the minimum distance between core and plane layers and R_1 the radius of curvature of the fiber. In this way, we take into account the curvature of the fiber while not needing to consider the cylindrical waveguide itself. According to all these considerations, we take as incident field

$$\mathbf{E_{inc}} = \frac{1}{N}\begin{bmatrix} \frac{K_0(\mathrm{WR})}{K_0(\mathrm{W})} \\ 0 \\ -j\frac{(2\Delta)^{1/2}}{V}W\frac{K_1(\mathrm{WR})}{K_0(\mathrm{W})} \end{bmatrix} \exp(j\beta z) \tag{2}$$

where R is the normalized radial coordinate (r/ρ, with ρ the core radius), which is calculated in our case taking into account (1), as

$$R = \sqrt{X^2 + Y^2} = \sqrt{\left(1 + \frac{D}{\rho}\right)^2 + \left(\frac{y}{\rho}\right)^2} \tag{3}$$

n_{cl} and n_{co} are the refractive indices of cladding and core, N is a normalization factor (corresponding to the total field transmitted in the fiber), $W = \rho\sqrt{\beta^2 - k_0^2 n_{\mathrm{cl}}^2}$ is the modal parameter of the cladding, $V = \rho\sqrt{k_0^2 n_{\mathrm{co}}^2 - k_0^2 n_{\mathrm{cl}}^2}$ is the normalized frequency of the fiber (k_0 is the vacuum wavenumber of the incident light and β is the propagation constant in the z direction), and $\Delta = \frac{1}{2}(1 - ((n_{\mathrm{cl}}^2)/(n_{\mathrm{co}}^2)))$ is the step-index factor. This field corresponds to a fundamental mode polarized along the x axis of the single mode fiber [17]

C. Calculation Procedure for the Field Distribution Determination

We use Rayleigh expansions of the field distribution in all the regions of the structure, starting with the one corresponding to the initial field. We establish relationships between the Fourier

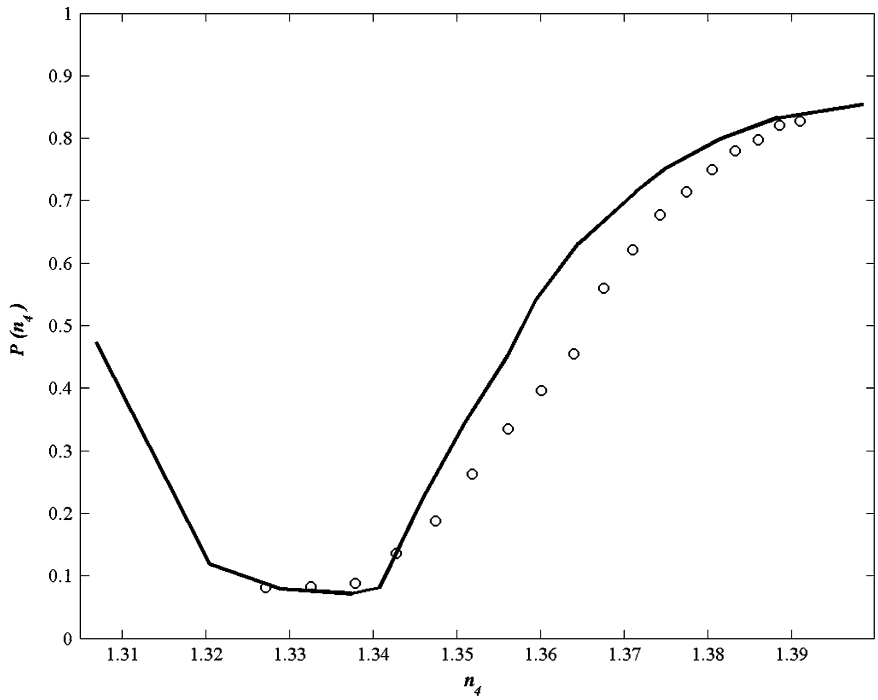

Fig. 3. Comparison between the prediction of the model (solid line) and experimental values (circles) for the dependence of the transmitted power P with the refractive index of the outer medium n_4. The data for the structure are Al, 8 nm; TiO_2, 60 nm; and minimum remaining cladding thickness 4.07 μm.

coefficients corresponding to each expansion by means of matrix equations obtained from the boundary conditions.

The relationship between the electric field vector and its Fourier components is given by

$$\mathbf{E}_m(x,y,z) = \frac{1}{4\pi^2}\int\int_{-\infty}^{\infty} e^{j(\nu y+\beta z)} \times \left[\mathbf{A}_m^+(\nu,\beta)e^{j\zeta_m x} + \mathbf{A}_m^-(\nu,\beta)e^{-j\zeta_m x}\right] d\nu d\beta. \quad (4)$$

Here, $\mathbf{A}_m^+$ and $\mathbf{A}_m^-$ are the vector Fourier amplitudes of the field in the mth medium, with the signs $\pm$ denoting the fields propagating in the positive and negative x directions, and ν and β are the components of the wave vector parallel to the interface (corresponding to the y and z coordinates). The third component of the wave vector (corresponding to the x direction, perpendicular to the interface), which varies in the different layers, can be related to ν and β by

$$\zeta_m = \left[k_0^2 n_m^2 - \nu^2 - \beta^2\right]^{1/2}. \quad (5)$$

The Fourier amplitudes are not independent, since the electric fields must fulfill the condition of zero divergence, which is equivalent to

$$\pm\zeta_m(\mathbf{A}_m^\pm)_x + \nu(\mathbf{A}_m^\pm)_y + \beta(\mathbf{A}_m^\pm)_z = 0. \quad (6)$$

We must also impose the constraint that no field is incoming to the multilayer from the outer medium

$$\mathbf{A}_m^-(\nu\beta) = 0. \quad (7)$$

The Fourier amplitudes in the different regions are related, because of the boundary conditions, by a matrix equation, in terms of the six vectors $(\mathbf{A}^+, \mathbf{A}^-)$

$$\begin{pmatrix}\mathbf{A}_{m+1}^+\\ \mathbf{A}_{m+1}^-\end{pmatrix} = \frac{1}{2\zeta_{m+1}}\begin{pmatrix}\mathbf{M}_{m,m+1}^{++} & \mathbf{M}_{m,m+1}^{+-}\\ \mathbf{M}_{m,m+1}^{-+} & \mathbf{M}_{m,m+1}^{--}\end{pmatrix}\begin{pmatrix}\mathbf{A}_m^+\\ \mathbf{A}_m^-\end{pmatrix} \quad (8)$$

for $m = 1, 2, \ldots, N-1$, where the 3×3 submatrices $\mathbf{M}_{m,m+1}^{\pm\pm}$ are directly obtained from the boundary conditions (developed form shown in [14]).

By applying this matrix equation we can obtain the Fourier amplitudes corresponding to any region in the structure, and, with an inverse Fourier transform operation, the field vector as a function of (y,z), thus permitting a complete determination of $\mathbf{E}(x,y,z)$ in the structure (the variation in x is trivial in each homogeneous layer and the continuity is assured by the matrix equation).

We can, of course, represent the values of our field distributions in any region and, in this way, visualize any of its characteristics and, specifically, surface plasmons (which will appear on the surface of the metallic layer). This is just a matter of numerical calculation.

D. Calculation of the Attenuation of the Guided Mode

Most sensors that are based on the studied structures use as a directly measurable parameter the output power of the fiber, which is affected somehow by a change in the working conditions, for instance, due to a variation of the refractive index of the surrounding medium. The fact that we have completely determined the field distribution over the whole structure makes it easy to estimate which will be the value of the power transmitted of the fiber once the interaction with the multilayer has happened. In this way, our theoretical method allows us to predict the measurable behavior of the sensors.

If we take into account that the basic loss mechanism in a surface-plasmon-resonance-based sensor will be the excitation of plasma waves, we can compute the energy that corresponds to the plasmon and simply subtract it from the power corresponding to the initial value of the field. Other loss mechanisms

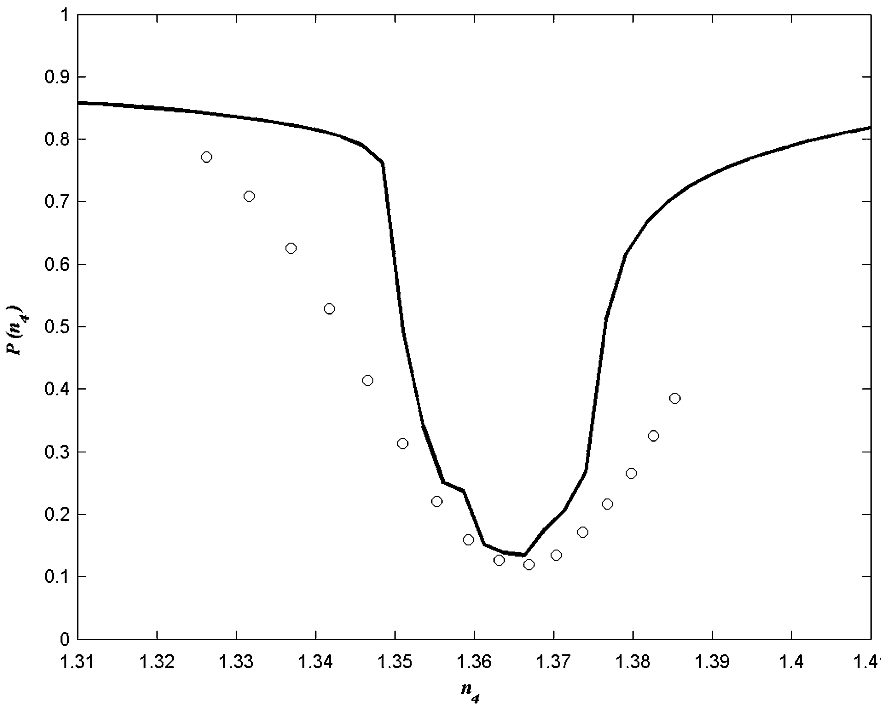

Fig. 4. Comparison between the prediction of the model (solid line) and experimental values (circles) for the dependence of the transmitted power P with the refractive index of the outer medium n_4. The data for the structure are Al, 8 nm; TiO_2, 47 nm; and minimum remaining cladding thickness 2.37 μm.

could be, however, taken into account quite easily by computing the energy associated to the field in other regions. The method is also versatile enough to be extended, for instance, to the case of rough surfaces, which can influence the surface plasmon fields, by introducing roughness parameters in the calculation.

Then, to theoretically model the performance of a surface-plasmon-resonance-based refractometer, we only need to iterate the calculations varying the parameter corresponding to the refractive index of the outer medium, n_N, obtain the field distribution in the metallic layer surface, compute the power associated to the surface plasmon and subtract it from the initial power (which has been normalized to 1), i.e.

$$P(n_N) = 1 - \left\langle \left|[\mathbf{E}(x_p, y, z)]\,(n_N)\right|^2 \right\rangle \tag{9}$$

where $< \cdots >$ indicates an spatial averaging (in the coordinates y, z) and x_p denotes the coordinate associated to the surface of the metallic layer where a plasmon can appear.

This is the equation we have used to compare the predictions of our method with the experimental results obtained with a real sensor. In this case, we *do* have the possibility of directly comparing experimental and theoretical curves, which cannot be done in most cases with other theoretical approaches, such as mode coupling.

III. Experimental Results

To prove the validity of the method for theoretically predicting the behavior of complex hybrid structures, we compare its prediction with the experimental results for a fiber-optic refractometer (used by us as a salinity meter, [4]) with the following configuration:

1) minimum remaining cladding thickness, $d_1 = 4.07\ \mu$m; refractive index of the cladding, $n_1 = 1.4528$;
2) metallic layer of aluminum, $d_2 = 8$ nm, $n_2 = 2.75 - 8.31j$;
3) dielectric layer of TiO_2, $d_3 = 60$ nm, $n_3 = 2.3$;
4) outer medium, semi-infinite, n_4 variable between 1.328–1.40;
5) light source with peak wavelength of 830 nm.

The results are shown in Fig. 3. The circles correspond to experimental measures and the continuous curve corresponds to the theoretical predictions of the method. The agreement is very good, and we can obtain the complete curve, not only the position of the "resonance" of the plasmon, which is usually what the methods based on mode-coupling give (and not always accurately). It is important, because the sensors must work with a dynamical range as wide as possible, detecting the values of the refractive index for, say, different concentrations of products in water (which is the way we varied the refractive index of the outer medium).

In Fig. 4, we show the results for a different configuration, with a titanium-dioxide layer of 47 nm and a minimum remaining cladding thickness of 2.37 μm (the rest of the parameters are unchanged). Again, the agreement is very good, even in this case, where we have a descending, as well as an ascending, portion of the curve, because of the displacement of the "resonance" to higher indices.

IV. Conclusion

In this work, we present a complete and detailed account of a theoretical method for the modeling of the behavior of hybrid guiding structures. These structures are commonly used as sensors, but the method is potentially applicable to many other situations, especially problems where plasmon generation is involved. The method not only gives us the distribution of the electric field as a three-dimensional function of the whole structure, but it can easily be used to compute the losses of the mode guided by the structure, which is a measurable parameter. The method does not rely on concepts like modes or coupling and, in this way, it is better suited for coping with problems associated with real systems, providing very good agreement with experiments, as we have shown with measures made with an operative fiber-optic refractometer.

The algorithms involved are simple and can easily be implemented in any mathematical software package; in our case, we have used MATLAB (MathWorks, Inc., Natick, MA).

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